Quantum hydrodynamic models for the two-band Kane system

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Summary. — We consider Kane's quantum model for two-band charged particles, composed of two Schrödinger-like equations coupled by a $k \cdot p$ term which describes interband tunneling. Using the WKB method we derive the hydrodynamic equations both for a zero-temperature and for a nonzero-temperature two-band quantum fluid. In the latter case, we introduce a family of closure relations and write in full details the simplest two-band, isentropic, fluid-dynamical model. Finally, introducing appropriate relaxation terms and performing drift-diffusive limits, we obtain the corresponding quantum drift-diffusion models for zero and nonzero-temperature quantum fluids.

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1. – Introduction

In recent years, much effort has been devoted to the study of hydrodynamic equations for new generations of semiconductor devices, for which quantum effects have to be taken into account. It is well known that fluid-dynamical models of semiconductors begin to fail when quantum phenomena become not negligible or even predominant. Nevertheless, the hydrodynamic approach presents notable advantages from the computational point of view.

In the classical framework, the literature on hydrodynamic models both from the theoretical and the numerical point of view is very wide. We refer the interested reader to one of the many review articles on the subject (see Anile *et al.* [1]).

Some very interesting results are present in literature, proposing quantum hydrodynamic equations, able to describe the behaviour of nanometric devices like resonant tunneling diodes. We recall here the "smooth" quantum hydrodynamic model proposed

by Gardner and Ringhofer [2], where the fluid-dynamical formulation is attained from moment expansion of a Wigner-Boltzmann equation and the approach by Jüngel [3], whose starting point is an appropriate representation of the solutions to the Schrödinger equation. A new derivation of quantum hydrodynamic models starting from first principles can be found in [4], where moments of the density matrix equation are considered and the resulting system is closed by an equilibrium density matrix.

The major part of published results is devoted to single-band problems. In the recent past new families of diodes, like Resonant Interband Tunneling Diodes (RITDs), have been produced, where the electrons in the valence band play an important role in the control of the current flow [5].

For such devices, we must consider the multi-band structure in the transport computation of the current. In this context, a simple model introduced by Kane [6] in the early 60's describes the electron behaviour in a system equipped with two allowed energy bands separated by a forbidden region. The Kane model is a simple two-band model capable of including one conduction band and one valence band in the device material and it is formulated as the coupling of two Schrödinger-like equations for the conduction and the valence band wave (envelope) functions [7]. The typical band diagram structure of a tunneling diode is characterized by a band alignment such that the valence band at the positive side of the semiconductor device lies above the conduction band at the negative one. The coupling term arises by the $k \cdot p$ perturbation method [8] using the fact that it is sufficient to obtain solutions of the single electron Schrödinger equation in the neighbourhood of the bottom of the conduction and the top of the valence bands, where the major part of electrons and holes, respectively, are concentrated. Such model is of great importance for RITD, and is widely used in literature [9,10].

The Kane model in the Schrödinger-like form has been recently studied by Kefi [11]. An alternative approach to study this model is the Wigner formulation of the Kane system [7]. Moreover the Kane model in his Wigner formulation can be used to obtain hydrodynamic models in terms of macroscopic quantities [12,13].

As we have said, the above-mentioned multiband models are based on the single electron Schrödinger equation, and the resulting equations are essentially linear. By applying the WKB method, it is possible to derive a zero-temperature hydrodynamic version of the Schrödinger Kane model. Although application of this method leads to nonlinear equations, for regular solutions the resulting quantum hydrodynamic equations are basically equivalent to the original linear quantum equations. However, when it is desirable to model the dynamics of a family of electrons, the quantum description requires the introduction of a sequence of mixed states, with attached a probability measure. In this case, the WKB method leads to a sequence of hydrodynamic equations, which are not satisfactory in real application. Anyway, it is possible to derive a set of equations for a finite number of macroscopic averaged quantities, with hydrodynamic character. These hydrodynamic equations share a similar structure with the analogous equation for a single electron, the only difference being the appearance of terms that can be interpreted as thermal tensors, and of additional source terms. These new terms depend on all states, so the system is not closed unless appropriate closure conditions are provided. It is clear that the final hydrodynamic model with temperature is by no means equivalent to the original quantum model. We could say that the nonlinearity of the resulting hydrodynamic model is "genuine" and is the price to pay for keeping only a finite number of equations.

In this paper, we describe in details this approach, by applying it to the Schrödinger Kane model for mixed states. The issues of closure relations is not discussed in full extent here, as it deserves an independent exposition. We limit ourselves to present the simplest

class of closure relations, based on some analogy with classical hydrodynamic models.

The paper is organized as follows. In sect. **2**, we review the Kane model and write it in nondimensional form. Then we introduce the hydrodynamic quantities needed to study a two-band quantum system. In sect. **4**, we obtain a system for the densities and the currents and we show how this system can be closed by a new equation for the phase difference. Such a system can be considered as the Madelung system for a two-band zero-temperature quantum fluid. Section **5** is devoted to the derivation of a nonzero-temperature model for the Kane system, by considering an electron ensemble represented by a mixed quantum-mechanical state. Then, in sect. **6**, introducing a relaxation time term, we perform the drift-diffusive limit, obtaining the corresponding quantum drift-diffusion system. Finally, a short discussion on this model and on related problems, such as closure and numerical implementation, is proposed.

2. – Physical description of the Kane model

The Kane model consists of a couple of Schrödinger-like equations for the conduction and the valence band envelope functions. It is used to describe the electron behaviour in a system equipped with two allowed energy bands separated by a forbidden region as a tunnel diode. The model is derived in the framework of the envelope function theory. In this approach the envelope function is a smooth function which can be obtained by replacing the wave function by its average in each primitive cell, since it is not necessary to find the exact evolution of the full wave equation.

Let $\psi_c(x,t)$ be the conduction band electron envelope function and $\psi_v(x,t)$ be the valence band electron envelope function, where $x \in \mathbb{R}^3$ is the space variable, and $t \in \mathbb{R}$ is the time. The Kane model reads as follows [6]:

$$(2.1) \qquad \begin{cases} i\hbar \dfrac{\partial \psi_c}{\partial t} &= -\dfrac{\hbar^2}{2m}\Delta\psi_c + V_c\psi_c - \dfrac{\hbar^2}{m}P\cdot\nabla\psi_v, \\[2mm] i\hbar \dfrac{\partial \psi_v}{\partial t} &= -\dfrac{\hbar^2}{2m}\Delta\psi_v + V_v\psi_v + \dfrac{\hbar^2}{m}P\cdot\nabla\psi_v. \end{cases}$$

Here, i is the imaginary unit, $\hbar$ is the Planck constant scaled by 2π, m is the bare mass of the carriers, V_c and V_v are the minimum of the conduction band energy and maximum of the valence band energy, respectively, and P is the coupling coefficient between the two bands. The coupling coefficient P is the matrix element of the gradient operator between the Bloch functions. It can be assumed to be real, and is given by

$$(2.2) \qquad P = \int_{u-\text{cell}} u_0^c(r)\nabla u_0^v(r)\mathrm{d}r\,,$$

where u-cell is the unitary cell and u_0^c and u_0^v are the basis of the Bloch functions for the conduction and valence bands, respectively, evaluated at the wave vector $k = 0$. In the Kane model the coupling parameter has to be considered constant. In realistic heterostructure semiconductor devices, the parameter P, approximatively expressed in terms of the effective electron mass and the energy gap, depends on the layer composition through the spatial coordinates.

In order to rewrite system (2.1) in a dimensionless form, we introduce the rescaled

Planck constant

$$\epsilon = \frac{\hbar}{\alpha},$$

where the dimensional parameter α is given by $\alpha = mx_R^2/t_R$, by using x_R and t_R as characteristic (scalar) length and time variables. We rescale system (2.1) to dimensionless units by introducing the scaled coordinates

$$t' = \frac{t}{t_R}, \ x' = \frac{x}{x_R},$$

and leaving the mass m unchanged. The band energy can be rescaled, taking new potential units $V_0 = mx_R^2/t_R^2$. A dimensional argument shows that the original coupling coefficient (2.2) is a reciprocal of a characteristic lenght, thus we define a scaled coefficient by $P' = Px_R$.

Hence, dropping the primes and without changing the name of the variables, we get the following scaled Kane system, which will be the object of our study:

(2.3)
$$\begin{cases} i\epsilon \dfrac{\partial \psi_c}{\partial t} &= -\dfrac{\epsilon^2}{2}\Delta\psi_c + V_c\psi_c - \epsilon^2 P \cdot \nabla\psi_v, \\[2mm] i\epsilon \dfrac{\partial \psi_v}{\partial t} &= -\dfrac{\epsilon^2}{2}\Delta\psi_v + V_v\psi_v + \epsilon^2 P \cdot \nabla\psi_c. \end{cases}$$

3. – The hydrodynamic quantities

The first aim of this paper is to derive the hydrodynamic version of system (2.3) using the WKB method. This is the classical approach to put the Schrödinger equation in hydrodynamic form [14]. It consists in characterizing the wave function by a quasi-classical limit expression $a \exp[iS/\epsilon]$, where a is called the amplitude and S/ϵ the phase of the wave. Using this approach the hydrodynamic limit is valid only for pure states, and in this sense, we say that the hydrodynamic limit is valid for a quantum system at zero temperature.

In the case under consideration of a two-band model, we look for solutions of the rescaled system (2.3) in the form

(3.1)
$$\begin{aligned} \psi_c(x,t) &= \sqrt{n_c(x,t)}\exp\left[\frac{iS_c(x,t)}{\epsilon}\right], \\[2mm] \psi_v(x,t) &= \sqrt{n_v(x,t)}\exp\left[\frac{iS_v(x,t)}{\epsilon}\right]. \end{aligned}$$

In the framework of the two-band Kane model, we introduce the particle densities

$$n_{ab} = \overline{\psi}_a \psi_b,$$

where ψ_a, with $a = c, v$, is the envelope function for the conduction and the valence band, respectively.

When $a = b$, the quantities $n_{ab} = n_a = |\psi_a|^2$ are real and represent the quantum probability densities for the position of conduction band and valence band electrons only in an approximate sense, because ψ_a are envelope functions which mix the Bloch states.

Nevertheless, $n = \overline{\psi}_c \psi_c + \overline{\psi}_v \psi_v$ is exactly the total electron density in conduction and valence band, and, as expected, satisfies a continuity equation.

When $a \neq b$, the density $\overline{\psi}_a \psi_b$ is a complex quantity, which does not have a precise physical meaning. Despite of this, as it will become clear in the next section, the complex quantities $\overline{\psi}_a \psi_b$ appear explicitly in the evolution equation for the total density n.

Looking for solutions in the form (3.1), it is natural to write the coupling terms in a more manageable way, by introducing the complex quantity

$$(3.2) \qquad n_{cv} := \overline{\psi}_c \psi_v = \sqrt{n_c} \sqrt{n_v}\, e^{i\sigma},$$

where σ is the phase difference defined by

$$(3.3) \qquad \sigma := \frac{S_v - S_c}{\epsilon}\,.$$

Now, it is apparent that, in order to study a zero-temperature quantum hydrodynamic model, we need to use only the three quantities n_c, n_v and σ to characterize the zero order moments (the "particle" densities).

The situation is more involved for the current densities. In analogy to the one-band case, we define quantum-mechanical electron current densities

$$J_{ab} = \epsilon\, \mathrm{Im}\, \left(\overline{\psi}_a \nabla \psi_b \right).$$

When $a = b$, using again the form (3.1), we recover the classical current densities

$$(3.4) \qquad J_c := \mathrm{Im}\, \left(\epsilon \overline{\psi}_c \nabla \psi_c \right) = n_c \nabla S_c, \quad J_v := \mathrm{Im}\, \left(\epsilon \overline{\psi}_v \nabla \psi_v \right) = n_v \nabla S_v\,,$$

whose physical meaning has to be interpreted similarly as for the particle densities. It is easy to get the identity

$$(3.5) \qquad \epsilon \overline{\psi}_a \nabla \psi_b = \sqrt{n_a} \sqrt{n_b} \exp\left[i \frac{S_b - S_a}{\epsilon} \right] \left(\epsilon \frac{\nabla \sqrt{n_b}}{\sqrt{n_b}} + i \nabla S_b \right)\,.$$

Also, we introduce the complex velocities u_c and u_v, with

$$(3.6) \qquad u_c := \frac{\epsilon \nabla \psi_c}{\psi_c} = \frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}} + i \nabla S_c, \quad u_v := \frac{\epsilon \nabla \psi_v}{\psi_v} = \frac{\epsilon \nabla \sqrt{n_v}}{\sqrt{n_v}} + i \nabla S_v.$$

We note that

$$(3.7) \qquad \epsilon \nabla n_{cv} = n_{cv}(\overline{u}_c + u_v).$$

The real and imaginary parts of u_c are called osmotic velocity and current velocity, respectively, and will be denoted by $u_{\mathrm{os},c}$ and the $u_{\mathrm{el},c}$. Explicitly we have

$$(3.8) \qquad u_{\mathrm{os},c} := \frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}}, \qquad u_{\mathrm{el},c} := \nabla S_c = \frac{J_c}{n_c}.$$

Analogous definitions hold for $u_{\mathrm{os},v}$ and $u_{\mathrm{el},v}$, so that

$$(3.9) \qquad\qquad u_c = u_{\mathrm{os},c} + iu_{\mathrm{el},c}, \quad u_v = u_{\mathrm{os},v} + iu_{\mathrm{el},v}.$$

Hence osmotic velocity and current velocity can be expressed solely in terms of n_c, n_v, J_c and J_v.

Coming back to the choice of the hydrodynamic quantities, we can maintain that for a zero-temperature quantum hydrodynamic system it is sufficient to take the usual quantities n_c, n_v, J_c and J_v, plus the phase difference σ. This will be verified in the next section.

4. – Hydrodynamic formulation of the Kane model

Taking into account the wave form (3.1) and using the first equation of the Kane system (2.3), we find

$$\frac{\partial n_c}{\partial t} = \overline{\psi}_c \frac{\partial \psi_c}{\partial t} + \psi_c \frac{\partial \overline{\psi}_c}{\partial t} = \frac{i\epsilon}{2} \left(\overline{\psi}_c \Delta \psi_c - \psi_c \Delta \overline{\psi}_c\right) + iP \cdot \left(\epsilon \overline{\psi}_c \nabla \psi_v - \epsilon \psi_c \nabla \overline{\psi}_v\right)$$
$$= -\nabla \cdot \operatorname{Im} \left(\epsilon \overline{\psi}_c \nabla \psi_c\right) - 2P \cdot \operatorname{Im} \left(\epsilon \overline{\psi}_c \nabla \psi_v\right).$$

In a similar way, we get

$$\frac{\partial n_v}{\partial t} = -\nabla \cdot \operatorname{Im} \left(\epsilon \overline{\psi}_v \nabla \psi_v\right) + 2P \cdot \operatorname{Im} \left(\epsilon \overline{\psi}_v \nabla \psi_c\right).$$

Using the definition of the particle densities and of the complex velocities, we find

$$(4.1) \qquad\qquad \epsilon \overline{\psi}_c \nabla \psi_v = n_{cv} u_v, \qquad \epsilon \overline{\psi}_v \nabla \psi_c = \overline{n}_{cv} u_c,$$

and then, recalling the definitions (3.4) of J_c and J_v, the previous equations become

$$(4.2) \qquad\qquad \begin{cases} \dfrac{\partial n_c}{\partial t} + \nabla \cdot J_c = -2P \cdot \operatorname{Im} \left(n_{cv} u_v\right), \\[2mm] \dfrac{\partial n_v}{\partial t} + \nabla \cdot J_v = 2P \cdot \operatorname{Im} \left(\overline{n}_{cv} u_c\right). \end{cases}$$

Explicitly, in terms of osmotic and current velocities, we can write

$$\begin{cases} n_{cv} u_v = \sqrt{n_c}\sqrt{n_v} \left(\cos \sigma + i \sin \sigma\right)(u_{\mathrm{os},v} + iu_{\mathrm{el},v}), \\[2mm] \overline{n}_{cv} u_c = \sqrt{n_c}\sqrt{n_v} \left(\cos \sigma - i \sin \sigma\right)(u_{\mathrm{os},c} + iu_{\mathrm{el},c}). \end{cases}$$

Summing the equations in (4.2) and using the identity $\operatorname{Im}\left(\epsilon \overline{\psi}_c \nabla \psi_v\right) - \operatorname{Im}\left(\epsilon \overline{\psi}_v \nabla \psi_c\right) = \epsilon \nabla \operatorname{Im} n_{cv}$, we obtain the balance law for the total density,

$$(4.3) \qquad\qquad \frac{\partial}{\partial t}(n_c + n_v) + \nabla \cdot (J_c + J_v) = -2\,\epsilon\,P \cdot \nabla \operatorname{Im} n_{cv}.$$

It is convenient to write eq. (4.3) in divergence form, in order to derive the conservation of total density. Using the fact that $\nabla \cdot P = 0$, (4.3) gives

$$\frac{\partial}{\partial t}(n_c + n_v) + \nabla \cdot (J_c + J_v + 2\epsilon P \operatorname{Im} n_{cv}) = 2\,\epsilon\,\operatorname{Im} n_{cv} \nabla \cdot P = 0\,,$$

which is just the quantum counterpart of the classical continuity equation.

We remark that $\nabla \cdot P = 0$ is obviously verified following the assumptions under which the Kane model is derived. On the other hand, the $k \cdot p$ approximation [8] which leads to the Kane model is performed under the assumption of null divergence. It is interesting to note that this assumption ensures the self-adjointness of the $k \cdot p$ Hamiltonian corresponding to the Schrödinger-type system (2.3).

Next, we derive equations for the phases S_c, S_v. Using (2.3) and (4.2), we have

$$\begin{aligned}
\frac{\partial S_c}{\partial t} &= -i\epsilon \frac{\partial}{\partial t} \ln\left(\frac{\psi_c}{\sqrt{n_c}}\right) \\
&= \frac{\epsilon^2}{2n_c}\left(\overline{\psi}_c \Delta \psi_c - i\nabla \cdot \operatorname{Im}\left(\overline{\psi}_c \nabla \psi_c\right)\right) - V_c + \frac{\epsilon^2}{n_c}P \cdot \left(\overline{\psi}_c \nabla \psi_v - i\operatorname{Im}\left(\overline{\psi}_c \nabla \psi_v\right)\right) \\
&= \frac{\epsilon^2}{2n_c}\left(\nabla \cdot \operatorname{Re}\left(\overline{\psi}_c \nabla \psi_c\right) - \nabla \overline{\psi}_c \cdot \nabla \psi_c\right) - V_c + \frac{\epsilon^2}{n_c}P \cdot \operatorname{Re}\left(\overline{\psi}_c \nabla \psi_v\right).
\end{aligned}$$

It is possible to rewrite the previous equation as

$$\frac{\partial S_c}{\partial t} = -\frac{1}{2}\left|\nabla S_c\right|^2 + \frac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} - V_c + \frac{\epsilon}{n_c}P \cdot \operatorname{Re}\left(\epsilon \overline{\psi}_c \nabla \psi_v\right).$$

A similar equation can be derived for S_v. Then, using (4.1), the resulting equations are

$$(4.4) \qquad \begin{cases} \dfrac{\partial S_c}{\partial t} + \dfrac{1}{2}\left|\nabla S_c\right|^2 - \dfrac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} + V_c = \dfrac{\epsilon}{n_c}P \cdot \operatorname{Re}\left(n_{cv} u_v\right), \\[4mm] \dfrac{\partial S_v}{\partial t} + \dfrac{1}{2}\left|\nabla S_v\right|^2 - \dfrac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} + V_v = -\dfrac{\epsilon}{n_v}P \cdot \operatorname{Re}\left(\overline{n}_{cv} u_c\right). \end{cases}$$

Equations (4.2) and (4.4) are equivalent to the coupled Schrödinger equations (2.3).

We would like to replace (4.4) with a system of coupled equations for the currents. Using the definitions (3.4), we can evaluate

$$(4.5) \qquad \frac{\partial J_c}{\partial t} = \sum_j \frac{\epsilon^2}{2}\frac{\partial}{\partial x_j}\operatorname{Re}\left(\overline{\psi}_c \nabla \frac{\partial \psi_c}{\partial x_j} - \nabla \psi_c \frac{\partial \overline{\psi}_c}{\partial x_j}\right) - \overline{\psi}_c \psi_c \nabla V_c +$$
$$+ \epsilon^2 \operatorname{Re}\left[\overline{\psi}_c \nabla(P \cdot \nabla \psi_v) - \nabla \psi_c(P \cdot \nabla \overline{\psi}_v)\right]\,.$$

To write this equation in terms of hydrodynamic quantities, we use the identities

$$\overline{\psi}_c \nabla \frac{\partial \psi_c}{\partial x_j} - \nabla \psi_c \frac{\partial \overline{\psi}_c}{\partial x_j} = \nabla\left(\overline{\psi}_c \frac{\partial \psi_c}{\partial x_j}\right) - 2\nabla\sqrt{n_c}\frac{\partial \sqrt{n_c}}{\partial x_j} - \frac{2n_c}{\epsilon^2}\nabla S_c \frac{\partial S_c}{\partial x_j},$$
$$\operatorname{Re}\nabla\left(\overline{\psi}_c \frac{\partial \psi_c}{\partial x_j}\right) = \frac{1}{2}\nabla\frac{\partial n_c}{\partial x_j},$$

with $j = 1, 2, 3$, which yield

$$\sum_j \frac{\partial}{\partial x_j} \operatorname{Re}\left(\overline{\psi}_c \nabla \frac{\partial \psi_c}{\partial x_j} - \nabla \psi_c \frac{\partial \overline{\psi}_c}{\partial x_j}\right) =$$
$$= \sum_j \frac{\partial}{\partial x_j}\left[\frac{1}{2}\nabla\frac{\partial n_c}{\partial x_j} - 2\nabla\sqrt{n_c}\frac{\partial\sqrt{n_c}}{\partial x_j} - \frac{2n_c}{\epsilon^2}\nabla S_c\frac{\partial S_c}{\partial x_j}\right].$$

Then, using

$$\operatorname{Re}\left[\overline{\psi}_c\nabla(P{\cdot}\nabla\psi_v) - \nabla\psi_c(P{\cdot}\nabla\overline{\psi}_v)\right] = \operatorname{Re}\left[\nabla(\overline{\psi}_c(P{\cdot}\nabla\psi_v)) - 2\nabla\overline{\psi}_c(P{\cdot}\nabla\psi_v)\right],$$

and the previous identities, eq. (4.5) becomes

(4.6) $$\frac{\partial J_c}{\partial t} + \operatorname{div}\left(\frac{J_c \otimes J_c}{n_c} + \epsilon^2\nabla\sqrt{n_c}\otimes\nabla\sqrt{n_c} - \frac{\epsilon^2}{4}\nabla\otimes\nabla n_c\right) +$$
$$+ n_c\nabla V_c = \epsilon^2\operatorname{Re}\left[\nabla(\overline{\psi}_c(P{\cdot}\nabla\psi_v)) - 2\nabla\overline{\psi}_c(P{\cdot}\nabla\psi_v)\right].$$

A similar equation can be written for J_v.

(4.7) $$\frac{\partial J_v}{\partial t} + \operatorname{div}\left(\frac{J_v \otimes J_v}{n_v} + \epsilon^2\nabla\sqrt{n_v}\otimes\nabla\sqrt{n_v} - \frac{\epsilon^2}{4}\nabla\otimes\nabla n_v\right) +$$
$$+ n_v\nabla V_v = -\epsilon^2\operatorname{Re}\left[\nabla(\overline{\psi}_v(P{\cdot}\nabla\psi_c)) - 2\nabla\overline{\psi}_v(P{\cdot}\nabla\psi_c)\right].$$

The left-hand sides of the equations for the currents can be put in a more familiar form by using the identity

$$\operatorname{div}\left(\nabla\sqrt{n_a}\otimes\nabla\sqrt{n_a} - \frac{1}{4}\nabla\otimes\nabla n_a\right) = -\frac{n_a}{2}\nabla\left[\frac{\Delta\sqrt{n_a}}{\sqrt{n_a}}\right], \quad a = c, v.$$

The correction terms

$$\frac{\epsilon^2}{2}\frac{\Delta\sqrt{n_a}}{\sqrt{n_a}}, \quad a = c, v,$$

can be identified with the quantum Bohm potentials for each band, in analogy with the single-band case. Moreover, using (4.1) and the identity

$$\epsilon^2\nabla\overline{\psi}_a(P{\cdot}\nabla\psi_b) = n_{ab}\,P{\cdot}u_b\,\overline{u_a}, \quad a, b = c, v,$$

the right-hand sides of eqs. (4.6) and (4.7) can be expressed in terms of the hydrodynamic quantities.

The resulting system takes the following form:

$$(4.8) \quad \begin{cases} \dfrac{\partial J_c}{\partial t} + \operatorname{div}\left(\dfrac{J_c \otimes J_c}{n_c}\right) - n_c \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V_c = \\ \qquad\qquad = -\epsilon\nabla \ \mathrm{Re}\ (n_{cv}P{\cdot}u_v) - 2\ \mathrm{Re}\ (n_{cv}P{\cdot}u_v\overline{u}_c)\,, \\[2mm] \dfrac{\partial J_v}{\partial t} + \operatorname{div}\left(\dfrac{J_v \otimes J_v}{n_v}\right) - n_v \nabla\left(\dfrac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V_v = \\ \qquad\qquad = -\epsilon\nabla \ \mathrm{Re}\ (\overline{n}_{cv}P{\cdot}u_c) + 2\ \mathrm{Re}\ (\overline{n}_{cv}P{\cdot}u_c\overline{u}_v)\,. \end{cases}$$

For the reader's convenience, we express the right-hand sides of (4.8) in terms of osmotic and current velocities:

$$\begin{cases} \mathrm{Re}\ (n_{cv}P{\cdot}u_v) &=& \sqrt{n_c}\sqrt{n_v}\ P{\cdot}(u_{\mathrm{os},v}\cos\sigma - u_{\mathrm{el},v}\sin\sigma)\,, \\[2mm] \mathrm{Re}\ (\overline{n}_{cv}P{\cdot}u_c) &=& \sqrt{n_c}\sqrt{n_v}\ P{\cdot}(u_{\mathrm{os},c}\cos\sigma + u_{\mathrm{el},c}\sin\sigma)\,, \\[2mm] \mathrm{Re}\ (n_{cv}P{\cdot}u_v\overline{u}_c) &=& \sqrt{n_c}\sqrt{n_v}\ [P{\cdot}(u_{\mathrm{os},c}\cos\sigma + u_{\mathrm{el},c}\sin\sigma)u_{\mathrm{os},v} - \\ && \qquad - P{\cdot}(u_{\mathrm{os},c}\sin\sigma - u_{\mathrm{el},c}\cos\sigma)u_{\mathrm{el},v}]\,, \\[2mm] \mathrm{Re}\ (\overline{n}_{cv}P{\cdot}u_c\overline{u}_v) &=& \sqrt{n_c}\sqrt{n_v}\ [P{\cdot}(u_{\mathrm{os},v}\cos\sigma - u_{\mathrm{el},v}\sin\sigma)u_{\mathrm{os},c} + \\ && \qquad + P{\cdot}(u_{\mathrm{os},v}\sin\sigma + u_{\mathrm{el},v}\cos\sigma)u_{\mathrm{el},c}]\,. \end{cases}$$

It is important to notice that, at variance with the uncoupled model, (4.2) and (4.8) are not equivalent to the original equation (2.3), due to the presence of σ. There are many ways to "close" the system, in order to obtain an extension of the classical Madelung fluid equations to a two-band quantum fluid. One possibility is to use (4.4) to derive an evolution equation for $\sigma = (S_v - S_c)/\epsilon$,

$$(4.9) \quad \epsilon\frac{\partial \sigma}{\partial t} - \frac{1}{2}\left|\frac{J_c}{n_c}\right|^2 + \frac{1}{2}\left|\frac{J_v}{n_v}\right|^2 + \frac{\epsilon^2 \Delta\sqrt{n_c}}{2\sqrt{n_c}} - \frac{\epsilon^2 \Delta\sqrt{n_v}}{2\sqrt{n_v}} -$$

$$-V_c + V_v = -\frac{\epsilon}{n_v}P{\cdot}\ \mathrm{Re}\ (\overline{n_{cv}}u_c) - \frac{\epsilon}{n_c}P{\cdot}\ \mathrm{Re}\ (n_{cv}u_v).$$

Equation (4.9) must be supplemented with the constraint

$$(4.10) \quad \epsilon\nabla\sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c}.$$

Using (4.2) and (4.8), it is possible to prove that (4.9) and (4.10) are equivalent, in the following sense: (4.9) implies that (4.10) is satisfied at all times if it holds at the initial time; (4.10) implies that (4.9) is satisfied (up to a constant).

To see the truth of the above statement, it is sufficient to take the gradient of (4.4) and, afterwards, account that

$$(4.11) \quad \nabla S_c = \frac{J_c}{n_c}, \qquad \nabla S_v = \frac{J_v}{n_v}.$$

Then, noting that (4.9) was derived from the same equation (4.4), it is simple to see that (4.9) implies

$$\frac{\partial}{\partial t}\left(\epsilon\nabla\sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c}\right) = 0,$$

which yields the first part of the statement. Similarly, taking the time derivative of (4.10) and using again (4.11), we can recover the gradient of equation (4.9), which implies the second part of the statement.

The equivalence of (4.10) and (4.9) suggests that we can discard (4.9), and recover σ as a function of the other variables by solving the elliptic equation

(4.12)
$$\epsilon\Delta\sigma = \nabla\cdot\left(\frac{J_v}{n_v} - \frac{J_c}{n_c}\right),$$

which can be obtained immediately after derivation of the constraint (4.10).

Another possibility is to regard n_{cv} as an independent variable, rather than σ. Recalling the definition (3.2) and Kane's system (2.3), we find

$$\frac{\partial n_{cv}}{\partial t} = \frac{i\epsilon}{2}\nabla\cdot\left(\overline{\psi}_c\nabla\psi_v - \psi_v\nabla\overline{\psi}_c\right) + \frac{i}{\epsilon}(V_c - V_v)\overline{\psi}_c\psi_v - i\epsilon P\cdot\left(\overline{\psi}_c\nabla\psi_c + \psi_v\nabla\overline{\psi}_v\right),$$

which, using (3.5) and the definitions of osmotic and current velocities, leads to

(4.13)
$$\epsilon\frac{\partial n_{cv}}{\partial t} = \frac{i\epsilon}{2}\nabla\cdot(n_{cv}(u_v - \overline{u}_c)) + i\,n_{cv}(V_c - V_v) - i\epsilon P\cdot(n_c u_c + n_v\overline{u}_v).$$

In addition to (4.13), the complex function n_{cv} must satisfy the constraints

(4.14) $$\overline{n}_{cv}n_{cv} = n_c n_v,$$
(4.15) $$\epsilon\nabla n_{cv} = (\overline{u}_c + u_v)n_{cv}.$$

Alternatively, we can use the identity (4.15) to derive a nonlinear elliptic equation for n_{cv},

(4.16)
$$\mathrm{div}\left(\frac{\epsilon\nabla n_{cv}}{n_{cv}}\right) = \mathrm{div}(\overline{u}_c + u_v),$$

which must be solved together with the constraint (4.14).

Now we are in position to rewrite the hydrodynamic system as follows:

$$(4.17) \quad \begin{cases} \dfrac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2P \cdot \, \mathrm{Im}\,(n_{cv} u_v), \\[2mm] \dfrac{\partial n_v}{\partial t} + \mathrm{div} J_v = \quad 2P \cdot \, \mathrm{Im}\,(\overline{n}_{cv} u_c), \\[2mm] \dfrac{\partial J_c}{\partial t} + \, \mathrm{div}\left(\dfrac{J_c \otimes J_c}{n_c}\right) - n_c \nabla\left(\dfrac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c \nabla V_c = \\[2mm] \qquad\qquad = \quad \epsilon \nabla \,\mathrm{Re}\,(n_{cv} P \cdot u_v) - 2\,\mathrm{Re}\,(n_{cv} P \cdot u_v \overline{u}_c)\,, \\[2mm] \dfrac{\partial J_v}{\partial t} + \, \mathrm{div}\left(\dfrac{J_v \otimes J_v}{n_v}\right) - n_v \nabla\left(\dfrac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v \nabla V_v = \\[2mm] \qquad\qquad = -\epsilon \nabla \,\mathrm{Re}\,(\overline{n}_{cv} P \cdot u_c) + 2\,\mathrm{Re}\,(\overline{n}_{cv} P \cdot u_c \overline{u}_v)\,, \\[2mm] \epsilon \nabla \sigma = \dfrac{J_v}{n_v} - \dfrac{J_c}{n_c}\,, \end{cases}$$

where n_{cv}, u_v, and u_v are expressed in the terms of the hydrodynamic quantities n_c, n_v, J_c, J_v, and σ by (3.2) and (3.9).

5. – Nonzero-temperature hydrodynamic model

In this section we extend the considerations of the previous sections to an ensemble of electrons, in order to obtain a nonzero-temperature model for the Kane system. An ensemble of electrons is represented by a mixed quantum-mechanical state, which is a sequence of single states with occupation probabilities λ_k for the k-th single state, $k = 0, 1, 2, \ldots$, described by the envelope function in the conduction band, ψ_c^k, and by the envelope function in the valence band, ψ_v^k. The occupation probabilities are such that $\sum_{k=0}^{\infty} \lambda_k = 1$.

The k-th state for the Kane system is described by the solutions of the system

$$(5.1) \quad \begin{cases} i\epsilon \dfrac{\partial \psi_c^k}{\partial t} &= \quad -\dfrac{\epsilon^2}{2}\Delta \psi_c^k + V_c \psi_c^k - \epsilon^2 P \cdot \nabla \psi_v^k\,, \\[3mm] i\epsilon \dfrac{\partial \psi_v^k}{\partial t} &= \quad -\dfrac{\epsilon^2}{2}\Delta \psi_v^k + V_v \psi_v^k + \epsilon^2 P \cdot \nabla \psi_c^k\,. \end{cases}$$

Using the Madelung-type transforms, under the assumption of positivity of the densities n_c^k and n_v^k,

$$\psi_c^k = \sqrt{n_c^k}\exp\left[iS_c^k/\epsilon\right]\,, \qquad \psi_v^k = \sqrt{n_v^k}\exp\left[iS_v^k/\epsilon\right]\,,$$

the previous system is equivalent to

$$(5.2) \quad \begin{cases} \dfrac{\partial n_c^k}{\partial t} + \operatorname{div} J_c^k = -2P \cdot \operatorname{Im}(n_{cv}^k u_v^k), \\[2mm] \dfrac{\partial n_v^k}{\partial t} + \operatorname{div} J_v^k = \quad 2P \cdot \operatorname{Im}(\overline{n_{cv}^k} u_c^k), \\[2mm] \dfrac{\partial J_c^k}{\partial t} + \operatorname{div}\left(\dfrac{J_c^k \otimes J_c^k}{n_c^k}\right) - n_c^k \nabla\left(\dfrac{\epsilon^2 \Delta \sqrt{n_c^k}}{2\sqrt{n_c^k}}\right) + n_c^k \nabla V_c = \\[2mm] \qquad\qquad = \quad \epsilon \nabla \operatorname{Re}(n_{cv}^k P \cdot u_v^k) - 2 \operatorname{Re}\left(n_{cv}^k P \cdot u_v^k \overline{u_c^k}\right), \\[2mm] \dfrac{\partial J_v^k}{\partial t} + \operatorname{div}\left(\dfrac{J_v^k \otimes J_v^k}{n_v^k}\right) - n_v^k \nabla\left(\dfrac{\epsilon^2 \Delta \sqrt{n_v^k}}{2\sqrt{n_v^k}}\right) + n_v^k \nabla V_v = \\[2mm] \qquad\qquad = -\epsilon \nabla \operatorname{Re}(\overline{n_{cv}^k} P \cdot u_c^k) + 2 \operatorname{Re}\left(\overline{n_{cv}^k} P \cdot u_c^k \overline{u_v^k}\right), \\[2mm] \epsilon \Delta \sigma^k = \nabla\left(\dfrac{J_v^k}{n_v^k} - \dfrac{J_c^k}{n_c^k}\right), \end{cases}$$

with

$$J_c^k = n_c^k \nabla S_c^k, \quad J_v^k = n_v^k \nabla S_v^k, \quad \sigma^k = \frac{S_v^k - S_c^k}{\epsilon},$$

$$n_{cv}^k = \sqrt{n_c^k}\sqrt{n_v^k}\exp\left[i\sigma^k\right],$$

$$u_c^k = \frac{\epsilon \nabla \sqrt{n_c^k}}{\sqrt{n_c^k}} + i\frac{J_c^k}{n_c^k}, \quad u_v^k = \frac{\epsilon \nabla \sqrt{n_v^k}}{\sqrt{n_v^k}} + i\frac{J_v^k}{n_v^k}.$$

The densities and the currents corresponding to the two mixed states for conduction and valence electrons can be defined as

$$n_c := \sum_{k=0}^{\infty} \lambda_k n_c^k, \quad n_v := \sum_{k=0}^{\infty} \lambda_k n_v^k,$$

$$J_c := \sum_{k=0}^{\infty} \lambda_k J_c^k, \quad J_v := \sum_{k=0}^{\infty} \lambda_k J_v^k.$$

We also define

$$\sigma := \sum_{k=0}^{\infty} \lambda_k \sigma^k, \quad n_{cv} := \sqrt{n_c}\sqrt{n_v}\exp[i\sigma],$$

$$u_c := \frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}} + i\frac{J_c}{n_c}, \quad u_v := \frac{\epsilon \nabla \sqrt{n_v}}{\sqrt{n_v}} + i\frac{J_v}{n_v}.$$

Multiplying (5.2) by λ_k and summing over k, we find

$$(5.3) \quad \begin{cases} \dfrac{\partial n_c}{\partial t} + \operatorname{div} J_c = -2P \cdot \operatorname{Im} R_c, \\[2mm] \dfrac{\partial n_v}{\partial t} + \operatorname{div} J_v = 2P \cdot \operatorname{Im} R_v, \\[2mm] \dfrac{\partial J_c}{\partial t} + \operatorname{div}\left(\dfrac{J_c \otimes J_c}{n_c} + n_c\theta_c\right) - n_c\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c\nabla V_c = \\[2mm] = \epsilon\nabla(P \cdot \operatorname{Re} R_c) - 2P \cdot \operatorname{Re} Q_{cv}, \\[2mm] \dfrac{\partial J_v}{\partial t} + \operatorname{div}\left(\dfrac{J_v \otimes J_v}{n_v} + n_v\theta_v\right) - n_v\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v\nabla V_v = \\[2mm] = -\epsilon\nabla(P \cdot \operatorname{Re} R_v) + 2P \cdot \operatorname{Re} Q_{vc}, \\[2mm] \epsilon\Delta\sigma = \nabla\left(\displaystyle\sum_{k=0}^{\infty}\lambda_k\left(\dfrac{J_v^k}{n_v^k} - \dfrac{J_c^k}{n_c^k}\right)\right), \end{cases}$$

with

$$R_c = \sum_{k=0}^{\infty}\lambda_k n_{cv}^k u_v^k, \qquad\qquad R_v = \sum_{k=0}^{\infty}\lambda_k \overline{n_{cv}^k} u_c^k,$$

$$Q_{cv} = \sum_{k=0}^{\infty}\lambda_k n_{cv}^k u_v^k \otimes \overline{u_c^k}, \qquad Q_{vc} = \sum_{k=0}^{\infty}\lambda_k \overline{n_{cv}^k} u_c^k \otimes \overline{u_v^k}.$$

Analogously to the one-band case [15], new terms containing the total temperature θ_c and θ_v, for each band, appear in the current equations. The temperature tensors $\theta_c = \theta_{\mathrm{os},c} + \theta_{\mathrm{el},c}$ and $\theta_v = \theta_{\mathrm{os},v} + \theta_{\mathrm{el},v}$ are the sum of osmotic temperature and electron current temperature, given by

$$\theta_{\mathrm{os},c} = \sum_{k=0}^{\infty}\lambda_k \frac{n_c^k}{n_c}(u_{\mathrm{os},c}^k - u_{\mathrm{os},c}) \otimes (u_{\mathrm{os},c}^k - u_{\mathrm{os},c}),$$

$$\theta_{\mathrm{el},c} = \sum_{k=0}^{\infty}\lambda_k \frac{n_c^k}{n_c}(u_{\mathrm{el},c}^k - u_{\mathrm{el},c}) \otimes (u_{\mathrm{el},c}^k - u_{\mathrm{el},c}).$$

We can write

$$(5.4) \qquad\qquad R_c = n_{cv}(\alpha u_v + \beta_v), \qquad R_v = \overline{n_{cv}}(\overline{\alpha}\, u_c + \beta_c),$$

with

$$\alpha := \sum_{k=0}^{\infty}\lambda_k \frac{n_{cv}^k}{n_{cv}}, \qquad \beta_v := \sum_{k=0}^{\infty}\lambda_k \frac{n_{cv}^k}{n_{cv}}(u_v^k - u_v), \qquad \beta_c := \sum_{k=0}^{\infty}\lambda_k \frac{\overline{n_{cv}^k}}{\overline{n_{cv}}}(u_c^k - u_c).$$

These quantities are not independent, due to (3.7). By taking the gradient of α, we find

$$(5.5) \qquad \epsilon \nabla \alpha - \beta_v - \overline{\beta_c} = -\alpha \left(\frac{\epsilon \nabla n_{cv}}{n_{cv}} - u_v - \overline{u_c} \right),$$

and using this identity, it is possible to show that $R_c + \overline{R_v} = \epsilon \nabla (\alpha n_{cv})$.
Moreover, recalling the definition of n_{cv}, u_c and u_v, we find

$$(5.6) \qquad \frac{\epsilon \nabla n_{cv}}{n_{cv}} - u_v - \overline{u_c} = i \left(\epsilon \nabla \sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c} \right).$$

Using this identity in (5.5), we get

$$\frac{1}{i\alpha} \left(\epsilon \nabla \alpha - \beta_v - \overline{\beta_c} \right) = -\epsilon \nabla \sigma + \frac{J_v}{n_v} - \frac{J_c}{n_c},$$

which implies

$$\mathrm{Re} \left\{ \frac{1}{\alpha} \left(\epsilon \nabla \alpha - \beta_v - \overline{\beta_c} \right) \right\} = 0,$$

$$\mathrm{Im} \left\{ \frac{1}{\alpha} \left(\epsilon \nabla \alpha - \beta_v - \overline{\beta_c} \right) \right\} = -\epsilon \nabla \sigma + \frac{J_v}{n_v} - \frac{J_c}{n_c}.$$

Next, in order to obtain an expression of the coupling terms between the two bands by a sort of temperature tensors, we write

$$Q_{cv} = n_{cv} \left(\alpha u_v \otimes \overline{u_c} + \beta_v \otimes \overline{u_c} + u_v \otimes \overline{\beta_c} + \theta_{cv} \right),$$
$$Q_{vc} = \overline{n_{cv}} \left(\overline{\alpha} u_c \otimes \overline{u_v} + \beta_c \otimes \overline{u_v} + u_c \otimes \overline{\beta_v} + \theta_{vc} \right),$$

with

$$\theta_{cv} := \sum_{k=0}^{\infty} \lambda_k \frac{n_{cv}^k}{n_{cv}} (u_v^k - u_v) \otimes (\overline{u_c^k} - \overline{u_c}),$$

$$\theta_{vc} := \sum_{k=0}^{\infty} \lambda_k \frac{\overline{n_{cv}^k}}{n_{cv}} (u_c^k - u_c) \otimes (\overline{u_v^k} - \overline{u_v}).$$

In conclusion, using the new quantities defined above, system (5.3) becomes

$$(5.7) \quad \begin{cases} \dfrac{\partial n_c}{\partial t} + \mathrm{div} J_c = -\, 2P\cdot \mathrm{Im}\,[n_{cv}\,(\alpha u_v + \beta_v)], \\[2mm] \dfrac{\partial n_v}{\partial t} + \mathrm{div} J_v = \quad 2P\cdot \mathrm{Im}\,[\overline{n_{cv}}\,(\overline{\alpha}\,u_c + \beta_c)], \\[2mm] \dfrac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\dfrac{J_c \otimes J_c}{n_c} + n_c\theta_c\right) - n_c\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c\nabla V_c = \\[2mm] \qquad\qquad = \ \epsilon\,P\cdot\nabla\,\mathrm{Re}\,(n_{cv}(\alpha u_v + \beta_v)) - \\[2mm] \qquad\qquad\qquad - 2P\cdot\mathrm{Re}\,\left(n_{cv}(\alpha u_v \otimes \overline{u_c} + \beta_v \otimes \overline{u_c} + u_v \otimes \overline{\beta_c} + \theta_{cv})\right), \\[2mm] \dfrac{\partial J_v}{\partial t} + \ \mathrm{div}\left(\dfrac{J_v \otimes J_v}{n_v} + n_v\theta_v\right) - n_v\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v\nabla V_v = \\[2mm] \qquad\qquad = -\epsilon\,P\cdot\nabla\,\mathrm{Re}\,(\overline{n_{cv}}\,(\overline{\alpha}u_c + \beta_c)) + \\[2mm] \qquad\qquad\qquad + 2P\cdot\mathrm{Re}\,\left(\overline{n_{cv}}\,(\overline{\alpha}u_c \otimes \overline{u_v} + \beta_c \otimes \overline{u_v} + u_c \otimes \overline{\beta_v} + \theta_{vc})\right), \\[2mm] \epsilon\nabla\sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = -\ \mathrm{Im}\left\{\dfrac{1}{\alpha}\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right)\right\}. \end{cases}$$

Unlike system (4.17), this system, which can be considered as a nonzero-temperature quantum fluid model, is not closed. The quantities n_{cv}, u_c, and u_v, already present in (4.17), are expressed in terms of n_c, n_v, J_c, J_v, and σ, while the new quantities α, β_c, and β_v are linked between them by

$$\mathrm{Re}\left\{\frac{1}{\alpha}\left(\epsilon\nabla\alpha - \beta_v - \overline{\beta_c}\right)\right\} = 0.$$

and need appropriate closure relations. Moreover, we must assign constitutive relations for the tensors θ_c, θ_v, θ_{cv} and θ_{vc}, the first ones formally analogous to the temperature tensor of kinetic theory.

A simple class of closure conditions can be obtained by assigning a function $\alpha = \alpha(n_c, n_v, \sigma)$ and taking

$$(5.8) \qquad \beta_c = 2n_c\frac{\partial\bar{\alpha}}{\partial n_c}u_{\mathrm{os},c} - \frac{\partial\bar{\alpha}}{\partial\sigma}u_{\mathrm{el},c}, \quad \beta_v = 2n_v\frac{\partial\alpha}{\partial n_v}u_{\mathrm{os},v} + \frac{\partial\alpha}{\partial\sigma}u_{\mathrm{el},v}.$$

Then, we have

$$\epsilon\nabla\alpha - \beta_v - \overline{\beta_c} = 0,$$

which implies

$$\epsilon\nabla\sigma - \frac{J_v}{n_v} + \frac{J_c}{n_c} = 0.$$

In particular, it is possible to choose

$$(5.9) \qquad\qquad\qquad \alpha = 1, \quad \beta_c = \beta_v = 0.$$

We still need to consider the temperature tensors θ_c, θ_v, θ_{cv} and θ_{vc}. Heuristically, following the analogy with the single-band fluid-dynamical model [3], the simplest closure relation is

(5.10) $$\theta_c = \frac{1}{n_c} p_c(n_c) I, \quad \theta_v = \frac{1}{n_v} p_v(n_v) I, \quad \theta_{cv} = \theta_{vc} = 0,$$

where I is the identity tensor and the functions p_c and p_v can be interpreted as pressures. In this way we obtain the simplest two-band, isentropic, fluid-dynamical model:

(5.11)
$$\begin{cases}
\dfrac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2P \cdot \mathrm{Im}\, (n_{cv}\, u_v), \\[2mm]
\dfrac{\partial n_v}{\partial t} + \mathrm{div} J_v = 2P \cdot \mathrm{Im}\, (\overline{n_{cv}}\, u_c), \\[2mm]
\dfrac{\partial J_c}{\partial t} + \mathrm{div} \left(\dfrac{J_c \otimes J_c}{n_c} + p_c(n_c) I \right) - n_c \nabla \left(\dfrac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) + n_c \nabla V_c = \\[2mm]
\qquad\qquad = \epsilon\, P \cdot \nabla\, \mathrm{Re}\, (n_{cv} u_v) - 2P \cdot \mathrm{Re}\, (n_{cv} u_v \otimes \overline{u_c}), \\[2mm]
\dfrac{\partial J_v}{\partial t} + \mathrm{div} \left(\dfrac{J_v \otimes J_v}{n_v} + p_v(n_v) I \right) - n_v \nabla \left(\dfrac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} \right) + n_v \nabla V_v = \\[2mm]
\qquad\qquad = -\epsilon\, P \cdot \nabla\, \mathrm{Re}\, (\overline{n_{cv}}\, u_c) + 2P \cdot \mathrm{Re}\, (\overline{n_{cv}}\, u_c \otimes \overline{u_v}), \\[2mm]
\epsilon \nabla \sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = 0.
\end{cases}$$

We remark that if the (classical) pressures are linear functions of n_c and n_v, respectively, then we reduce to the so-called isothermal case.

6. – The drift-diffusive scaling

In kinetic theory of gases, it is customary to introduce a relaxation-time term in order to simulate the mechanisms which force the system towards the statistical mechanical equilibrium. In semiconductor physics, the collisional mechanisms are more intricate and difficult to simulate by simple phenomenological models. Anyway, also in this case, it is classical to introduce momentum and energy relaxation times.

First, we consider a modified version of the single state system (4.17), with additional relaxation terms for the currents, by rewriting the current equations as

(6.1)
$$\begin{cases}
\dfrac{\partial J_c}{\partial t} + \mathrm{div} \left(\dfrac{J_c \otimes J_c}{n_c} \right) - n_c \nabla \left(\dfrac{\epsilon^2 \Delta \sqrt{n_c}}{2\sqrt{n_c}} \right) + n_c \nabla V_c = \\[2mm]
\qquad\qquad = \epsilon \nabla\, \mathrm{Re}\, (n_{cv} P \cdot u_v) - 2\, \mathrm{Re}\, (n_{cv} P \cdot u_v \overline{u}_c) - \dfrac{J_c}{\tau}, \\[2mm]
\dfrac{\partial J_v}{\partial t} + \mathrm{div} \left(\dfrac{J_v \otimes J_v}{n_v} \right) - n_v \nabla \left(\dfrac{\epsilon^2 \Delta \sqrt{n_v}}{2\sqrt{n_v}} \right) + n_v \nabla V_v = \\[2mm]
\qquad\qquad = -\epsilon \nabla\, \mathrm{Re}\, (\overline{n}_{cv} P \cdot u_c) + 2\, \mathrm{Re}\, (\overline{n}_{cv} P \cdot u_c \overline{u}_v) - \dfrac{J_v}{\tau}.
\end{cases}$$

Here τ is a relaxation time, which we assume equal for the two bands.

In analogy with the classical diffusive limit for a one-band system [3], we introduce the following (diffusive) scaling:

$$(6.2) \qquad t \to \frac{t}{\tau}, \quad J_c \to \tau J_c, \quad J_v \to \tau J_v \,.$$

Consequently, from definition (3.3), the phase difference has to be rescaled in such a way that

$$\epsilon \nabla \sigma = \frac{J_v}{n_v} - \frac{J_c}{n_c} \to \tau \frac{J_v}{n_v} - \tau \frac{J_c}{n_c} = \tau \epsilon \nabla \sigma \,.$$

This simple consideration leads to the ansatz

$$\sigma \to \sigma_0 + \tau \sigma \,,$$

where σ_0 is a constant phase to be determined. Then, we have

$$
\begin{aligned}
n_{cv} &\to \sqrt{n_c}\,\sqrt{n_v}\,e^{i\sigma_0} + i\sqrt{n_c}\,\sqrt{n_v}\,e^{i\sigma_0}\sigma\tau + O(\tau^2), \\
u_c &\to \frac{\epsilon \nabla \sqrt{n_c}}{\sqrt{n_c}} + i\frac{\tau J_c}{n_c}, \\
u_v &\to \frac{\epsilon \nabla \sqrt{n_v}}{\sqrt{n_v}} + i\frac{\tau J_v}{n_v}.
\end{aligned}
$$

Using these relations, for the coupling terms we find

$$
\begin{aligned}
n_{cv} u_v &\to \sqrt{n_c}\sqrt{n_v}\,e^{i\sigma_0} u_{\mathrm{os},v} \quad + i\sqrt{n_c}\sqrt{n_v}\,e^{i\sigma_0}\left(\sigma u_{\mathrm{os},v} + u_{\mathrm{el},v}\right)\tau \ + O(\tau^2)\,, \\
\overline{n_{cv}} u_c &\to \sqrt{n_c}\sqrt{n_v}\,e^{-i\sigma_0} u_{\mathrm{os},c} - i\sqrt{n_c}\sqrt{n_v}\,e^{-i\sigma_0}\left(\sigma u_{\mathrm{os},c} - u_{\mathrm{el},c}\right)\tau + O(\tau^2)\,.
\end{aligned}
$$

According to the previous scaling, up to the first order in τ, the balance equations for the densities become

$$(6.3) \qquad
\begin{cases}
\tau\left\{\dfrac{\partial n_c}{\partial t} + \mathrm{div}\,J_c\right\} = -2\sqrt{n_c}\sqrt{n_v}\,\sin\sigma_0 P{\cdot}u_{\mathrm{os},v}- \\[2mm]
\qquad -\tau\left\{2\sqrt{n_c}\sqrt{n_v}\,\cos\sigma_0\left(\sigma P{\cdot}u_{\mathrm{os},v} + P{\cdot}u_{\mathrm{el},v}\right)\right\} + O(\tau^2), \\[3mm]
\tau\left\{\dfrac{\partial n_v}{\partial t} + \mathrm{div}\,J_v\right\} = -2\sqrt{n_c}\sqrt{n_v}\,\sin\sigma_0 P{\cdot}u_{\mathrm{os},c}- \\[2mm]
\qquad -\tau\left\{2\sqrt{n_c}\sqrt{n_v}\,\cos\sigma_0\left(\sigma P{\cdot}u_{\mathrm{os},c} - P{\cdot}u_{\mathrm{el},c}\right)\right\}.
\end{cases}
$$

Formally, as τ tends to zero, the previous equations give $\sin\sigma_0 = 0$, that is, $\sigma_0 = 0$. Using this value, as τ tends to zero, the limit equations of (6.3) take the form

$$(6.4) \qquad
\begin{cases}
\dfrac{\partial n_c}{\partial t} + \mathrm{div}\,J_c = -2\sqrt{n_c}\sqrt{n_v}\left(\sigma P{\cdot}u_{\mathrm{os},v} + P{\cdot}u_{\mathrm{el},v}\right)\,, \\[3mm]
\dfrac{\partial n_v}{\partial t} + \mathrm{div}\,J_v = -2\sqrt{n_c}\sqrt{n_v}\left(\sigma P{\cdot}u_{\mathrm{os},c} - P{\cdot}u_{\mathrm{el},c}\right)\,.
\end{cases}
$$

Finally, performing the previous scaling on the current equations and expressing the osmotic and current velocities in terms of the other hydrodynamic quantities, the hydro-dynamic system will be formally reduced to

(6.5)
$$
\begin{cases}
\dfrac{\partial n_c}{\partial t} + \mathrm{div}J_c = -2\epsilon\sigma\sqrt{n_c}\,P\!\cdot\!\nabla\sqrt{n_v} - 2\dfrac{\sqrt{n_c}}{\sqrt{n_v}}\,P\!\cdot\!J_v, \\[2mm]
\dfrac{\partial n_v}{\partial t} + \mathrm{div}J_v = -2\epsilon\sigma\sqrt{n_v}\,P\!\cdot\!\nabla\sqrt{n_c} + 2\dfrac{\sqrt{n_v}}{\sqrt{n_c}}\,P\!\cdot\!J_c, \\[2mm]
J_c = n_c\,\nabla\!\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) - n_c\nabla V_c + \\[2mm]
\qquad + \epsilon^2\nabla\left(\sqrt{n_c}\,P\!\cdot\!\nabla\sqrt{n_v}\right) - 2\epsilon^2 P\!\cdot\!\nabla\sqrt{n_v}\,\nabla\sqrt{n_c}\,, \\[2mm]
J_v = n_v\nabla\!\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) - n_v\nabla V_v - \\[2mm]
\qquad - \epsilon^2\nabla\left(\sqrt{n_v}\,P\!\cdot\!\nabla\sqrt{n_c}\right) + 2\epsilon^2 P\!\cdot\!\nabla\sqrt{n_c}\,\nabla\sqrt{n_v}\,, \\[2mm]
\epsilon\nabla\sigma = \dfrac{J_v}{n_v} - \dfrac{J_c}{n_c}\,.
\end{cases}
$$

This system represents the analog of the zero-temperature quantum drift-diffusion model for the Kane system.

We can use the same procedure to perform the diffusive limit of the non-zero temperature system (5.7). As before, we consider a modified version of system (5.7), with additional relaxation terms for the currents. Using the closure relation (5.8), we rewrite (5.7) as

(6.6)
$$
\begin{cases}
\dfrac{\partial n_c}{\partial t} + \mathrm{div}J_c = -2P\!\cdot\!\mathrm{Im}\left[n_{cv}\left(\alpha u_v + \beta_v\right)\right], \\[2mm]
\dfrac{\partial n_v}{\partial t} + \mathrm{div}J_v = \ \ \ 2P\!\cdot\!\mathrm{Im}\left[\overline{n_{cv}}\left(\overline{\alpha}\,u_c + \beta_c\right)\right], \\[2mm]
\dfrac{\partial J_c}{\partial t} + \ \mathrm{div}\left(\dfrac{J_c\otimes J_c}{n_c} + n_c\theta_c\right) - n_c\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) + n_c\nabla V_c = \\[2mm]
\qquad = \ \epsilon\,P\!\cdot\!\nabla\,\mathrm{Re}\,\left(n_{cv}(\alpha u_v + \beta_v)\right) - \\[2mm]
\qquad\quad - 2P\!\cdot\!\mathrm{Re}\,\left(n_{cv}(\alpha u_v\otimes\overline{u_c} + \beta_v\otimes\overline{u_c} + u_v\otimes\overline{\beta_c} + \theta_{cv})\right) - \dfrac{J_c}{\tau}, \\[2mm]
\dfrac{\partial J_v}{\partial t} + \ \mathrm{div}\left(\dfrac{J_v\otimes J_v}{n_v} + n_v\theta_v\right) - n_v\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) + n_v\nabla V_v = \\[2mm]
\qquad = -\epsilon\,P\!\cdot\!\nabla\,\mathrm{Re}\,\left(\overline{n_{cv}}\left(\overline{\alpha}u_c + \beta_c\right)\right) + \\[2mm]
\qquad\quad + 2P\!\cdot\!\mathrm{Re}\,\left(\overline{n_{cv}}\left(\overline{\alpha}u_c\otimes\overline{u_v} + \beta_c\otimes\overline{u_v} + u_c\otimes\overline{\beta_v} + \theta_{vc}\right)\right) - \dfrac{J_v}{\tau}, \\[2mm]
\epsilon\nabla\sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = 0.
\end{cases}
$$

As done for the zero-temperature system, we introduce the (diffusive) scaling (6.2) which again leads to the ansatz $\sigma \to \sigma_0 + \tau\sigma$, where σ_0 is a constant phase to be

determined. Moreover, we assume that

$$\alpha \to \alpha_0 + \tau\alpha, \quad \alpha_0 = \overline{\alpha_0}.$$

A justification of this ansatz can be found by inspecting the definition of α in terms of the mixed densities of the simple states n_{cv}^k. Basically, we are assuming that for all k we have $\sigma^k \to \sigma_0 + \tau\sigma^k$, for the same σ_0. As a result, the first term of the expansion of α around $\tau = 0$ is real.

Then, proceeding as for the zero-temperature system, we find $\sigma_0 = 0$ and

$$(6.7) \quad \begin{cases} \dfrac{\partial n_c}{\partial t} + \mathrm{div} J_c = -2\sqrt{n_c}\sqrt{n_v}\left(\alpha_v \sigma P \cdot u_{\mathrm{os},v} + \alpha_0 P \cdot u_{\mathrm{el},v}\right), \\[2mm] \dfrac{\partial n_v}{\partial t} + \mathrm{div} J_v = -2\sqrt{n_c}\sqrt{n_v}\left(\alpha_c \sigma P \cdot u_{\mathrm{os},c} - \alpha_0 P \cdot u_{\mathrm{el},c}\right), \\[2mm] J_c = -\,\mathrm{div}\left(n_c\theta_c\right) + n_c\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_c}}{2\sqrt{n_c}}\right) - n_c\nabla V_c + \\[2mm] \qquad + \epsilon\, P \cdot \nabla\left(\sqrt{n_c}\sqrt{n_v}\alpha_v u_{\mathrm{os},v}\right) - 2\sqrt{n_c}\sqrt{n_v}\left(\alpha_{cv}P \cdot u_{\mathrm{os},v}u_{\mathrm{os},c} + P \cdot \mathrm{Re}\,\theta_{cv}\right), \\[2mm] J_v = -\,\mathrm{div}\left(n_v\theta_v\right) + n_v\nabla\left(\dfrac{\epsilon^2\Delta\sqrt{n_v}}{2\sqrt{n_v}}\right) - n_v\nabla V_v - \\[2mm] \qquad - \epsilon\, P \cdot \nabla\left(\sqrt{n_c}\sqrt{n_v}\alpha_c u_{\mathrm{os},c}\right) + 2\sqrt{n_c}\sqrt{n_v}\left(\alpha_{cv}P \cdot u_{\mathrm{os},c}u_{\mathrm{os},v} + P \cdot \mathrm{Re}\,\theta_{vc}\right), \\[2mm] \epsilon\nabla\sigma - \dfrac{J_v}{n_v} + \dfrac{J_c}{n_c} = 0, \end{cases}$$

with

$$\alpha_c := \alpha_0 + 2n_c\frac{\partial\alpha_0}{\partial n_c}, \quad \alpha_v := \alpha_0 + 2n_v\frac{\partial\alpha_0}{\partial n_v}, \quad \alpha_{cv} := \alpha_0 + 2n_c\frac{\partial\alpha_0}{\partial n_c} + 2n_v\frac{\partial\alpha_0}{\partial n_v}.$$

7. – Concluding remarks

In this paper we have applied the WKB method in order to rewrite the two-band, Schrödinger-like, Kane's system in terms of conduction and valence band electron densities and currents n_c, n_v, J_c and J_v. The strict analogies with the single-band case have allowed us to define the osmotic and current velocities as complex quantities which can be expressed solely by means of n_c, n_v, J_c and J_v. In addition, the coupling term n_{cv} has been defined by introducing the phase difference σ. Then, we have obtained the hydrodynamic equations for a zero-temperature two-band quantum fluid in the form (4.17), using the usual quantities n_c, n_v, J_c and J_v, plus the phase difference σ.

The extension to mixed quantum-mechanical state has given rise to the nonzero-temperature quantum hydrodynamic system (5.7), which is not closed. The closure of this system can be achieved by different methods: in this paper we have limited ourselves to recall the isentropic and the isothermal assumptions.

As we have already said in the introduction, quantum hydrodynamic models can be derived using different approaches, but the classical WKB method has the advantage of handling directly mathematical quantities, which can be easily extended to the two-band case, still keeping a specific physical meaning.

The results presented in this work are only formal and the mathematical analysis needs further investigations. In particular existence, uniqueness or non-uniqueness of the solutions to such models need to be studied.

In this paper we have also performed the diffusive limit and we have deduced the corresponding quantum drift-diffusion system.

The future research is oriented towards a physically-based closure of the hydrodynamic system and towards the numerical validation of the drift-diffusion model.

<div align="center">* * *</div>

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